Efficient Combustion Chemistry for Gas Turbine Combustor Simulations

Stephen B. Pope (pope@mae.cornell.edu; 607-255-4314)
Vivek Saxena (saxena@mae.cornell.edu; 607-255-4379)
Cornell University
Sibley School of Engineering
Upson Hall, Ithaca, NY 14853

M.S. Anand (iemsa@agt.gmeds.com; 317-230-2828)
Allison Engine Company
Speed Code T-14
2001 S. Tibbs Avenue
Indianapolis, IN 46241

Abstract

This abstract describes the background and objectives of the research program, which at the time of writing, had been underway for two months.

Introduction

In an advanced gas turbine combustor, the combustion of the fuel takes place in a highly turbulent flow. To be useful as an analytical design tool, a turbulent combustion model has to be able to calculate not only the mean flow and temperature fields, but also the generation and subsequent reaction of pollutants such as NO_X, CO, and unburned hydrocarbones (UHC). The accuracy of the design tool is critical to the reliable prediction of important combustor performance parameters, such as efficiency, emissions, exit and wall temperatures, ignition, lean blowout, and stability.

The probability density function (PDF) approach is the most suited method for such flows, since in this method, arbitrarily complex (non-linear, finite-rate, coupled) reactions can be treated without modeling assumptions (Pope 1990). Conventional Reynolds-average modeling approaches, on the other hand, cannot treat such reactions that typically occur in turbulent combustion without restrictive and often unrealistic and erroneous assumptions.

PDF methods have been developed at Cornell and applied to a variety of relatively simple flows, such as wakes, jets, mixing layers, one-dimensional premixed flames (e.g., Anand & Pope 1987), and jet diffusion flames (e.g., Norris & Pope 1995). Allison, in collaboration with the PI, has developed and validated the joint PDF method for more complex flows in its ongoing efforts to develop the method as a gas turbine combustor design tool. The method has been successfully used to compute recirculating, swirling, reacting, and particle-laden flows representing the important features of gas turbine combustor flows (e.g., Anand et al. 1996).

A most valuable advance in recent years has been the development of detailed chemical kinetics schemes for hydrocarbon fuels and NO_X chemistry. Notable in the context of natural gas combustion are the GRI mechanisms for methane combustion. The mechanism GRI-Mech 2.11, consisting of 49 species and 282 reactions, includes the nitrogen chemistry related to NO_X. Without doubt, this scheme is sufficiently comprehensive to address nearly all the issues related to gas-phase natural gas combustion.

PDF methods can treat complex reactions without modeling approximations, and detailed mechanisms for natural gas are available. But, used in conjunction, the computational cost is prohibitive. To realize the potential of PDF methods combined with realistic chemistry, a computer implementation of the chemistry that is faster by at least a factor of 10,000 is required, and can be achieved through the proposed research.

The approach to be used and further developed in this program is the ISAT algorithm (in situ adaptive tabulation, Pope 1997). In some applications, this method has already demonstrated a speed-up of over 1,000.

Research Objectives

The principle objectives of the research work are:

1. To develop a methodology for the efficient implementation of combustion chemistry that (a) can be applied to any detailed mechanism, (b) is efficient with controlled accuracy, and (c) requires minimal human effort to apply.

2. To test thoroughly the accuracy and computational efficiency of the methodology with different relevant reaction mechanisms for simple flows under different thermodynamics conditions.

3. To use the methodology in conjunction with the existing PDF code to make calculations of lean premixed combustion in combustor geometries for which there are benchmark quality experimental data.

Status

At Cornell, the ISAT algorithm is being further tested, both for a partially stirred reactor, and in conjunction with the PDF code. The algorithm has been transferred to Allison, where it will be tested in their combustor-design code.

References

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Cornell University
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Engineering

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2001 S. Tibbs Ave., Indianapolis, IN 46241

RESEARCH AREA: COMBUSTION

Contract:	DE-FC21-92MC29061
DOE COR:	William F. Geer, Jr.
Subcontract:	96-01-SR049
Program Manager:	Daniel B. Fant
Contractor:	Cornell University
Subcontractor:	Allison Engine Company
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OBJECTIVES

Context

- Advanced Turbine System performance depends crucially on the combustor performance
- Computational tools play a central role in the design of combustors
- Detailed chemistry computations---essential for modelling pollutants (e.g., NO_x and CO) extinction etc.---are prohibitively expensive using existing approaches

OBJECTIVES

- To develop a methodology for the efficient implementation of detailed combustion chemistry which
  - can be applied to any detailed mechanism
  - is efficient with controlled accuracy
  - requires minimal human effort to apply
- To test thoroughly the methodology with different mechanisms for simple flows under different thermodynamical conditions
- To use the methodology in existing PDF code for lean premixed combustion in combustor geometries for which there are benchmark quality experimental data

RELEVANCE

The research will aid the development of efficient combustor design tools. The new methodology addresses the following ATS industry needs:

- Reliable prediction of performance parameters for combustors, e.g.,
  - efficiency
  - exit and wall temperature
  - ignition, lean blow out and stability
- Accurate predictions of the generation of pollutants such as NO_x, CO and UHC

METHODOLOGY

Approach

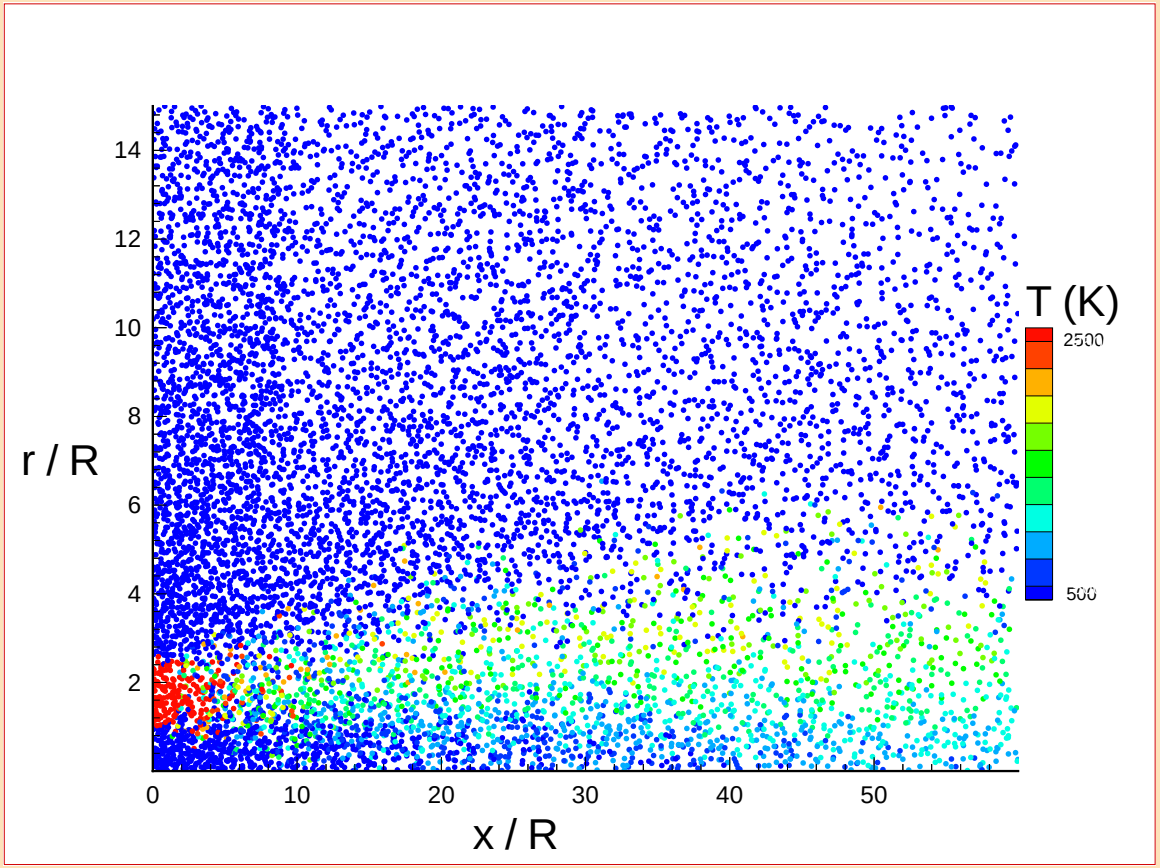
- Solve for the joint probability density function (JPDF) of velocity-frequency-composition
- Compute chemistry efficiently using the technique of *in situ* adaptive tabulation (ISAT).
- Our approach of coupling the joint PDF method with the new chemistry algorithm (ISAT) is unique
- No other methodology currently exists to compute detailed combustion chemistry with comparable accuracy and efficiency

ACCOMPLISHMENTS

The JPDF-ISAT calculations of a test flame--a piloted jet diffusion flame of methane--have been accomplished

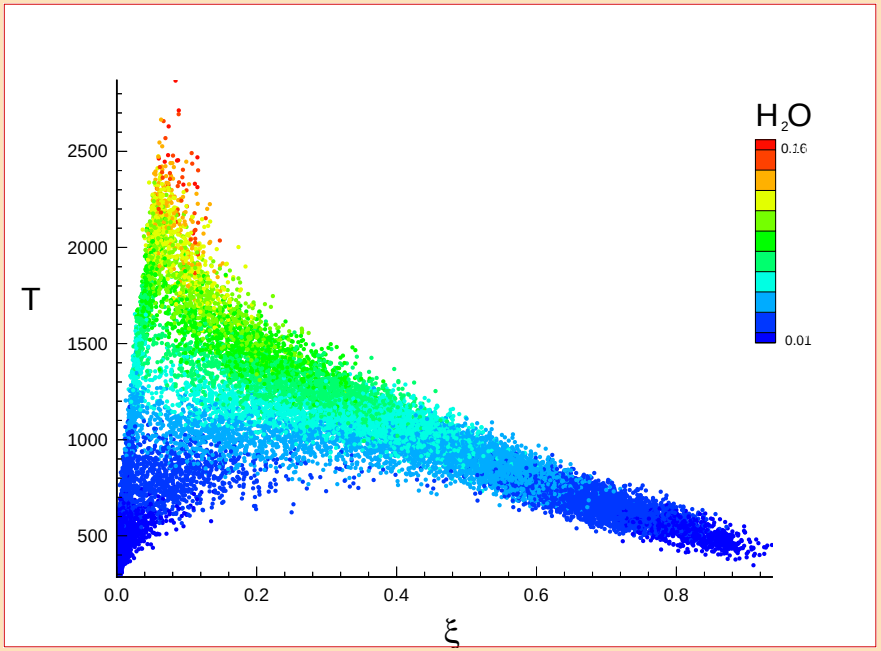
- Experimental data: Flame ‘L’ from Sydney University and Sandia Nat’l Lab. experiments
- Chemistry: 16 species-41 reaction skeletal mechanism
- A typical calculation requires
  - 10 hours of CPU time on an SGI Indigo 2 Workstation
  - 10 Mbytes of storage for ISAT

Scatter Plots of Temperature Over the Whole Domain

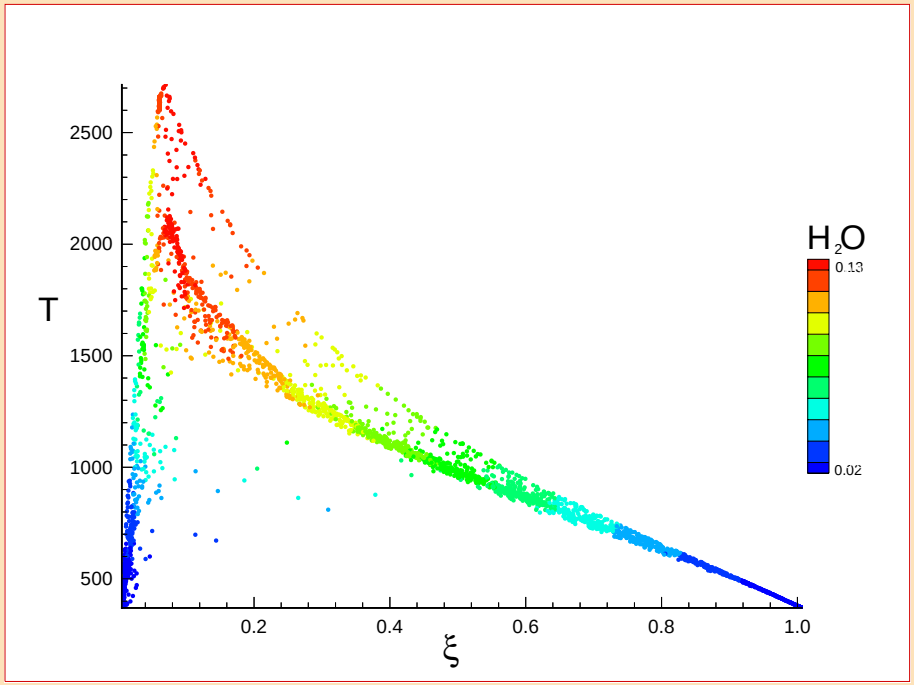


PILOTED METHANE JET FLAME

EXPERIMENT: MASRI ET AL (1988)



JPDF CALCULATION



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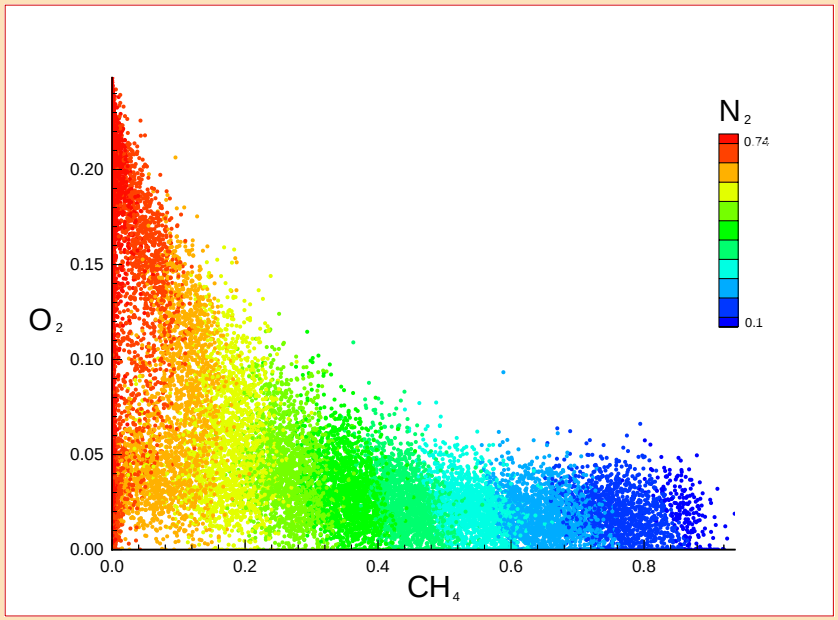

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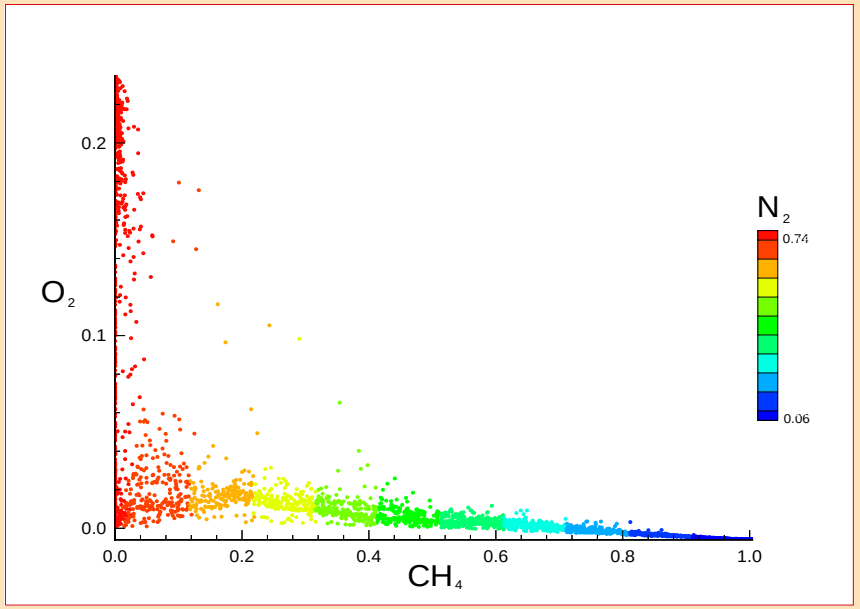

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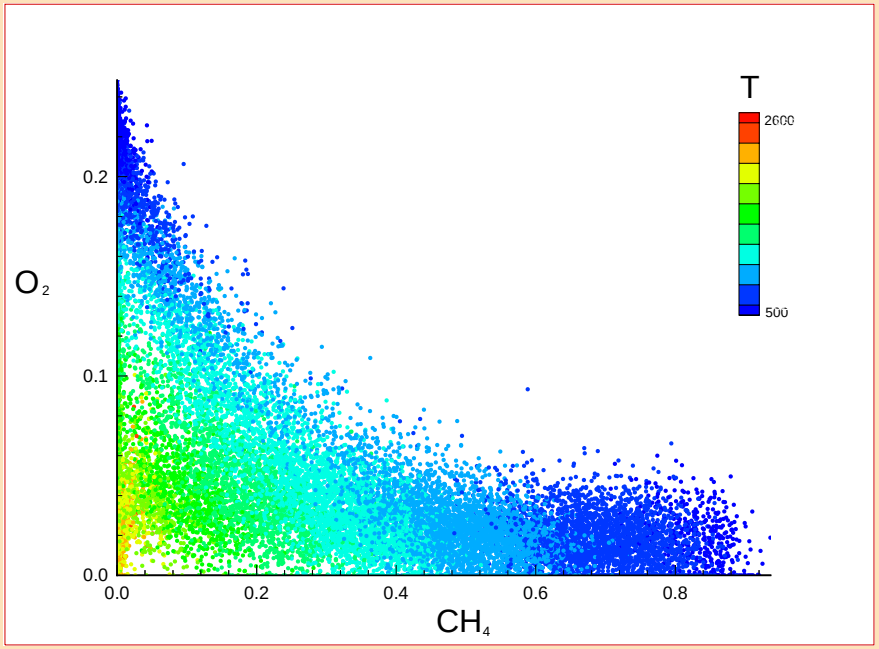
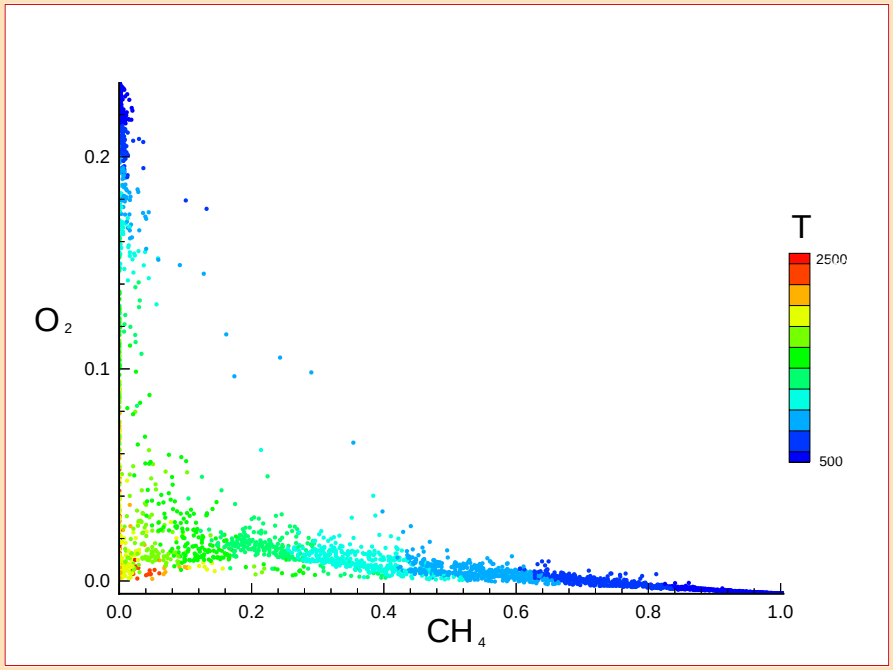


JPDF CALCULATION



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COLLABORATION

- Industry
  - Jun Xu, a Cornell graduate student, had an AGTSR internship at Allison Engine Company in 1997
  - Allison Engine Company is using the JPDF code developed at Cornell
  - Allison Engine Company is also using the ISAT code developed at Cornell
- Academia
  - Brigham Young University: Dr. Steve Cannon used ISAT for his thesis work on computing lean premixed combustion

CONCLUSIONS

Results

- Routine calculations of detailed combustion chemistry are now possible using the ISAT approach with a JPDF code
- The JPDF calculations with ISAT technique show controlled accuracy and acceptable CPU time requirements
- Detailed comparison with standard laboratory flames are currently underway

Future Work

- Further developments of the ISAT technique, particularly in reducing table dimensionality
- Calculation for realistic combustor geometries
- More comparisons with benchmark data
- Sensitivity studies for different models for mixing, turbulence and chemistry